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Quantum Lattice-Gas Automata and Hydrodynamics

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Abstract

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This document is the final report for AFOSR Grant F49620-01-1-385, "Quantum Lattice-Gas Automata and Hydrodynamics." Under the terms of this grant, the Department of Mathematics at Tufts University provided theoretical and computational support to the Quantum Computation group at the Air Force Research Laboratory at Hanscom AFB. The principal research topics were the development of quantum lattice-gas models for implementation on Type II quantum computers, and classical entropic lattice Boltzmann models. The work was conducted at the level of three months FTE per year for three years. Eight publications and twelve invited presentations have resulted from the work conducted under effort. The principal results of this work are described in this report.

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1 Principal Areas of Study

1.1 Entropic Lattice Boltzmann Models

Lattice Boltzmann models of viscous, incompressible fluid dynamics evolve a single-particle distribution function in discrete time steps on a regular spatial lattice. The velocity space is also discrete and, in the simplest instance, consists of the lattice vectors themselves. The simplest variety of lattice Boltzmann models employs a collision operator of Bhatnager-Gross-Krook (BGK) form, with a specified collisional relaxation time, τ .

Such models take advantage of the fact that the Boltzmann equation is generally more forgiving to extreme discretization than are the Navier-Stokes equations which derive from them. The lattice Boltzmann equation is fully explicit, and requires no upwind differencing or other such artifices. Yet, using the Chapman-Enskog analysis, it is possible to show that the mass and momentum moments of the distribution function can be made to satisfy the Navier-Stokes equation to any desired accuracy.

The viscosity that appears in the Navier-Stokes equations obtained from these models is proportional to $\tau - \frac{1}{2}$. To lower viscosity and thereby increase Reynolds number, practitioners often over-relax the collision operator by using values of τ in the range $(\frac{1}{2}, 1]$. For sufficiently small τ , however, the method loses numerical stability, and this consideration limits the highest Reynolds numbers attainable.

To address this stability problem, *entropic lattice Boltzmann models* were invented by Boghosian and Yezep [1] as work performed under the earlier AFOSR Grant F49620-99-1-0070, and independently by at least one other group [2, 3]. These models are motivated by the observation that the loss of stability is due to the absence of an H theorem [1]. Numerical instabilities evolve in ways that would be precluded by the existence of a Lyapunov function. The idea behind entropic lattice Boltzmann models is to specify an H function, rather than just the form of the equilibrium. Of course, the equilibrium distribution will be that which extremizes the H function. The evolution will be required never to decrease H , yielding a rigorous discrete-time H -theorem, and an absolutely stable dynamical model.

To ensure that collisions never decrease H , the collision time τ is made a function of the incoming state by solving for the smallest value $\tau_{\min} < 1$ that does not increase an imposed Lyapunov function H . The value then used is $\tau = \tau_{\min}/\kappa$ where $0 < \kappa < 1$. It has been shown that the expression for the viscosity obtained by the Chapman-Enskog analysis will approach zero as κ approaches unity [1]. Thus, the entropic lattice Boltzmann methodology allows for arbitrarily low viscosity together with a rigorous discrete-time H theorem, and concomitant absolute stability. The upper limit to the Reynolds numbers attainable by the model is therefore determined by loss of resolution of the smallest eddies, rather than by loss of stability [1, 4, 5].

What had not been known was how to choose the form of the H function so that the entropic lattice Boltzmann program would yield the Navier-Stokes equations correctly. Under AFOSR grant F49620-01-1-385, we answered this question in a sequence of three papers [6, 7, 8]. Two of these constructed entropic lattice Boltzmann models for the Navier-Stokes equations in two and three dimensions, and thereby addressed Tasks 1.1, and 1.3 of our proposal for AFOSR grant F49620-01-1-385. The third constructed an entropic lattice Boltzmann model for Burgers equation.

We showed that the requirement of Galilean invariance of the resulting model – specifically, the correct form for the convective derivative operator – makes the choice of H function unique. We also showed that the required function has the form of the Burg entropy in two dimensions, and the Tsallis entropy in higher dimensions. To demonstrate this, we assumed that the H function could be written in trace form

$$H = \sum_{\mathbf{x}} \sum_j h(f_j(\mathbf{x})),$$

where h is to be determined. The local equilibrium distribution is then the solution to the extremization problem

$$0 = \frac{\partial}{\partial f_i} \left[\sum_j h(f_j) - \Gamma_\rho \sum_j f_j - \Gamma_{\mathbf{u}} \cdot \sum_j \mathbf{v}_j f_j \right],$$

where the Γ 's are Lagrange multipliers, designed to preserve the mass and momentum moments of the distribution. The local equilibrium is then

$$f_i^{\text{eq}} = \phi(\Gamma_\rho + \Gamma_{\mathbf{u}} \cdot \mathbf{v}_i)$$

where $\phi = h'^{-1}$; that is, the form of the equilibrium is the inverse function of the first derivative of h . By using this local equilibrium as the unperturbed problem in the Chapman-Enskog expansion in D spatial dimensions, we showed that the resulting Navier-Stokes equations for the hydrodynamic velocity \mathbf{u} are

$$\frac{\partial \mathbf{u}}{\partial t} + \left(\frac{D}{D+2} \right) \frac{\phi(x)\phi''(x)}{[\phi'(x)]^2} \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u}.$$

It should be noted that the theory for doing this was worked out by Love and Boghosian [9] during the period of this grant. It is clear that these are correct if and only if $\phi\phi'' = (1 + \frac{2}{D})(\phi')^2$, so that the coefficient in front of the convective term is unity. This differential equation yields determines the form of the H function uniquely. The details of this calculation are presented in [6]; the extension of the argument to multi-speed lattice Boltzmann models is presented in [7].

Entropic lattice Boltzmann models have generated considerable interest since their inception. Indeed, Chen, Succi and Orszag [10] have suggested that they may constitute a new class of subgrid models for large eddy simulation. Such models continue to decrease a Lyapunov function even when the smallest turbulent eddies are smaller than can be resolved by the computational grid, and this is tantamount to a dissipation model for the smallest eddies. To investigate this further, the Tufts and AFRL group constructed an entropic lattice Boltzmann model for Burgers equation [8]. This model compared favorably to the Cole-Hopf solution to Burgers equation as long as the width of the Burgers shock remained large compared to the lattice spacing; when this was no longer true, the simulation results exhibited oscillations of bounded amplitude in the vicinity of the shock. Thus, while the Lyapunov function precluded instability, the sharp gradients excited parasitic “ghost modes” that reduced the accuracy of the solution. The question of how large one may make the Knudsen number in these kinds of simulations without unacceptable loss of accuracy is still very much open, and is likely to be an important topic of research in coming years.

1.2 High-Performance Computing Cluster

Task 1.2 of our proposal indicated that we would create a high-performance computing cluster in the Department of Mathematics at Tufts University. Thanks to AFOSR Grant F49620-01-1-385, as well as AFOSR Grant F49620-01-1-0456, we were able to achieve this goal. We purchased a Beowulf cluster in early 2002, with nine dual-processor Athlon boxes, clocked at 1.4 GHz, each with 2 Gb of memory and an 18 Gb SCSI disk drive. The processors are connected with a gigabit ethernet network, supplied by Tufts University. The machine is housed in a rack in Tufts Data Center, protected by UPS and halon, as well as by security personnel. We have used this machine for all of the simulations conducted under this Grant, as described in Task 1.3 of our proposal.

Our computational resources were supplemented by the recent donation of an 8-processor UltraSPARC machine in early 2004. We have cited our ability to operate and maintain a large, heterogeneous cluster in a series of successful NSF grants for large allocations of computer time that we use for classical CFD studies of vortex dynamics.

1.3 Type II Quantum Lattice Models

Type II quantum lattice models were first advanced by Yepez at AFRL at Hanscom AFB. They are lattice models in which the collision outcomes are computed quantum mechanically, but measured before being streamed classically. This measurement means that different lattice sites are never entangled, and that the scaling of computational complexity with the lattice size is just the same as it is in a classical lattice model. The difference is that the quantum computation of the collision outcome allows for the use of collision operators that give rise to exceedingly low viscosities; these collision operators would be much too difficult to implement on any classical computer.

For example one of the original lattice-gas models of two-dimensional hydrodynamics employed a triangular lattice in two dimensions, with anywhere from zero to six particles at each site. The presence or absence of each particle is encoded as a bit of information, the state of one site is represented by six bits, and therefore 2^6 such states are possible. The discrete single-particle distribution function may then be represented by six real numbers, each representing the average occupation number of its corresponding bit. The lattice-gas collision operator can be written in terms of bits using Boolean operations, and these may in turn be represented by nonlinear numerical operations. For example, if a and b are numerical representations of Boolean variables, such that 0/1 means false/true, then the AND operation on a and b may be written as the product ab , and the OR operation is $a + b - ab$. Written in this way, each of the 6 components of the collision operator may have up to 2^6 terms. If the underlying lattice-gas model satisfies detailed balance, then it may be shown that the corresponding lattice Boltzmann model, obtained by ensemble averaging the lattice-gas collision operator, possesses a Lyapunov function. In a sense, it is therefore an entropic lattice Boltzmann model. Like other entropic lattice Boltzmann models, it allows for small values of the viscosity, and concomitantly high values of Reynolds number. Unfortunately, it is a particularly difficult lattice Boltzmann model to implement on a classical computer.

To see the origin of the difficulty, recall that the simplest lattice-gas models of three-dimensional fluids require, not six, but 24 bits per site. The collision operator will then have

24 components, each of which may have up to 2^{24} terms. This number is large enough that it is not possible to compute the outcome of the collision operator at each lattice site in this manner using current computer hardware. If extra velocities or species are included, this number of bits may easily double or triple, in which case no current *or even contemplated* computer hardware is up to the task.

Type II quantum algorithms get around this difficulty by applying a unitary operator to the state of each site on the lattice. They then measure the outcome on an ensemble of quantum computers; such an ensemble is provided naturally by nuclear magnetic resonance machines. If the state is represented by b classical bits, then b quantum bits may represent a complex superposition of the 2^b possible states. A unitary operation on these 2^b states would require on the order of 2^{2b} calculations on a classical computer; it may be accomplished with a number of quantum gates that is polynomial in b . This observation addresses Task 1.7 of the proposal.

In previous work, Boghosian and Yepez studied the transition from lattice-gas to lattice Boltzmann models by letting the number of bits/particles associated with each direction be greater than one [11]. In the work conducted under this grant, they, along with Peter Love of Tufts University, used this approach to relate Type II quantum lattice algorithms to entropic lattice Boltzmann models. In fact, they succeeded in showing that all Type II quantum lattice algorithms are indeed lattice Boltzmann models. As part of Grant F49620-01-1-385, Yepez and Boghosian worked out efficient quantum lattice models for the many-body Schrödinger equation [12]. Recently, Yepez, Vahala and Vahala worked out a Type II quantum lattice algorithm for the equations of magnetohydrodynamics in one spatial dimension. This model appears to be remarkably robust, and exhibits no parasitic “ghost modes,” even when the magnetic Reynolds number is made very high. It is not well understood why the Type II algorithm performs so robustly when entropic lattice Boltzmann algorithms exhibit the ghost modes. This remains an active and ongoing area of research.

Likewise, a perfectly general Type II algorithm that may be specified without enumerating the state space of a site is a goal of ongoing research.

2 Conclusions

We have described the program of activity of the lattice-gas research collaboration between the Tufts University Department of Mathematics and the Quantum Computation group at AFRL at Hanscom AFB. This collaboration has centered on the development of entropic lattice Boltzmann models and Type II quantum lattice models. We have provided a detailed account of the principal new results in both of these areas. Eight publications and numerous presentations have resulted from this effort. These, along with the PI’s recent honors and awards, are described in the appendices.

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A Publications

The following publications, coauthored by Bruce M. Boghosian, resulted from AFOSR Grant F49620-01-1-385, and were published in refereed journals during the time period of the grant:

1. Bruce M. Boghosian, Peter J. Love, Jeffrey Yepez, "Entropic lattice Boltzmann model for Burgers's equation," *Phil. Trans.: Math., Phys. & Eng. Sci.* **362** (2004) 1691-1701.
2. Peter J. Love, Bruce M. Boghosian, "Quaternionic Madelung Transformation and Non-abelian Fluid Dynamics," to appear in *Physica A* **332** (2004) 47-59.
3. Peter J. Love, Bruce M. Boghosian, David A. Meyer, "Lattice-Gas Simulations of Dynamical Geometry in One Dimension," *Phil. Trans. Roy. Soc. A*, to appear (2004).
4. Bruce M. Boghosian, Peter J. Love, Jeffrey Yepez, "Galilean-Invariant Multi-speed Entropic Lattice Boltzmann Models," *Physica D* **193** (2003) 169-181.
5. Peter J. Love, Bruce M. Boghosian, "On the Dependence of the Navier Stokes Equations on the Distribution of Molecular Velocities," *Physica D* **193** (2003) 182-194.
6. Bruce M. Boghosian, Peter J. Love, Peter Coveney, Sauro Succi, Ilya Karlin, Jeffrey Yepez, "Galilean-Invariant Lattice Boltzmann Models with H-Theorem," *Phys. Rev. E Rapid Communications* **68** (2): Art. No. 025103 Part 2 (2003).
7. Bruce M. Boghosian, Peter J. Love, David A. Meyer, "Toward the Simplest Hydrodynamic Lattice-Gas Model," *Philosophical Transactions of Proc. Roy. Soc. Lon.* **360** (2002) 333-344.
8. Jeffrey Yepez, Bruce M. Boghosian, "An Efficient and Accurate Quantum Lattice-Gas Model for the Many-Body Schrodinger Wave Equation," *Comp. Phys. Comm.* **146** (2002) 280-294.

B Invited Talks and Presentations

The following invited talks and presentations by Bruce M. Boghosian resulted from AFOSR Grant F49620-01-1-385, and were presented during the time period of the grant:

1. Speaker, SC Global, Supercomputing 2003 (20 November 2003). Winner of HPC Challenge Award for Most Innovative Data-Intensive Application.
2. Speaker, RealityGrid Annual Conference, Royal Society of London (17-18 June 2003).
3. Speaker, AFOSR Grantees Meeting, University of Florida, Graduate Engineering Research Center (29-30 May 2003).
4. Speaker, Quantum Information Processing (QIP) Colloquium, Massachusetts Institute of Technology (10 March 2003).
5. Speaker, Workshop on Anomalous Distributions, Nonlinear Dynamics, and Nonextensivity, Center for Nonlinear Studies, Los Alamos National Laboratory, Santa Fe, New Mexico (7 November 2002).
6. Speaker, Greater Boston Statistical Physics Workshop, Brandeis University, Waltham, Massachusetts (19 October 2002).
7. Session Chair, New England Complex Systems Institute, Annual Meeting, Nashua, New Hampshire (11 June 2002).
8. Speaker, Department of Electrical, Computer and Systems Engineering, Boston University, Boston, Massachusetts (15 May 2002).
9. Speaker, Workshop on Quantum Computing for Physical Modeling, Martha's Vineyard, Massachusetts (9 May 2002).
10. Lecturer, "Joint MIT-Harvard-BU Lecture Series on Theoretical Chemistry," (9 January 2002).
11. Speaker, Knowledge Foundation Conference on Mesoscale Modelling, Boston, Massachusetts (13-14 August 2001).
12. Member of Topical Committee for sessions on dynamical systems and turbulence, Stat-Phys 21 Meeting, Cancun, Mexico (15-20 July 2001).
13. Speaker, "Tenth International Conference on Discrete Models for Fluid Dynamics" Cargese, Corsica (1-7 July, 2001).

C Honors and Awards

Bruce Boghosian was a co-recipient of the High Performance Computing (HPC) Challenge award for Most Innovative Data-Intensive Computation presented at the Supercomputing 2003 conference, sponsored by the Association for Computing Machinery (2003).

Bruce Boghosian received the Undergraduate Initiative in Teaching (UNITE) award from the College of Arts, Sciences and Engineering, Tufts University (2002).

Bruce Boghosian remains on the editorial advisory boards of *Physica A*, the *International Journal of Modern Physics C*, and *Computers in Science and Engineering*.